Quantized Berry Phases for a Local Characterization of Spin Liquids in Frustrated Spin Systems ‡

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Abstract. Recently by using quantized Berry phases, a prescription for a local characterization of *gapped* topological insulators is given[1]. One requires the ground state is gapped and is invariant under some anti-unitary operation. A spin liquid which is realized as a unique ground state of the Heisenberg spin system with frustrations is a typical target system, since pairwise exchange couplings are always time-reversal invariants even with frustrations.

As for a generic Heisenberg model with a finite excitation gap, we locally modify the Hamiltonian by a continuous $SU(2)$ twist only at a specific link and define the Berry connection by the derivative. Then the Berry phase evaluated by the entire many-spin wavefunction is used to define the local topological order parameter at the link. We numerically apply this scheme for several spin liquids and show its physical validity.

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1. Topological Orders

In a modern condensed matter physics, a concept of the symmetry breaking has a fundamental importance. At a sufficiently low temperature, most of classical systems show some ordered structure which implies that the symmetry at the high temperature is spontaneously lost or reduced. This is the spontaneous symmetry breaking which is usually characterized by using a *local* order parameter as an existence of the long range order. States of matter in a classical system are mostly characterized by this order parameter with the symmetry breaking. Even in a quantum system, the local order parameter and the symmetry breaking play similar roles and they form a foundation of our physical understanding. Typical examples can be ferromagnetic and Neel orders in spin systems.

Recent studies in decades have revealed that this symmetry breaking may not be always enough to characterize some of important quantum states[2, 3]. Low dimensionality of the system and/or geometrical frustrations come from the strong correlation can prevent from a formation of the local order. Especially with a quantum fluctuation, there may happen that a quantum ground state without any explicit symmetry breaking is realized even in the zero temperature. Such a state is classified as a quantum liquid which mostly has an energy gap (may not be always). Typical example of this quantum liquids is the Haldane spin chain and the valence bond solid (VBS) states[4, 5]. Also some of the frustrated spin systems and spin-Peierls systems can belong to this class[6, 7, 8]. To characterize these quantum liquids, a concept of a topological order can be useful[2, 3]. It was proposed to characterize quantum Hall states which are typical quantum liquids with energy gaps. There are many clearly different quantum states but they do not have any local order parameter associated with symmetry breaking. Then topological quantities such as a number of degenerate ground states and the Chern numbers as the Hall conductance are used to characterize the quantum liquids. We generalize the idea to use the topological quantities such as the Chern numbers for the characterization of the generic quantum liquids[3]. This is a global characterization. When we apply this to spin systems with the time-reversal symmetry (TR), the Chern number is vanishing in most cases. Recently we propose an alternative for the system with the TR invariance by the quantized Berry phases[1]. Although, the Berry phases can take any values generically, the TR invariance of the ground state guarantees a quantization of the Berry phases which enables us to use them as local topological order parameters. In the present article, we use it for several spin systems with frustrations and verify the validity. Although the geometrical frustration affects the standard local order substantially, it does not bring any fundamental difficulties for the topological characterizations as shown later. It should be quite useful for characterizations for general quantum liquids[1].

Finally we mention on the energy spectra of the systems with classical or topological orders. There can be interesting differences between the standard order and the topological order. As for energy spectra, we have two situations when the symmetry is

spontaneously broken. If the spontaneously broken symmetry is continuous, there exists a gapless excitation as a Nambu-Goldstone mode. On the other hand, the symmetry is discrete, the ground states are degenerate and above these degenerate states, there is a finite energy gap. Note that when the system is finite (with periodic boundary condition), the degeneracy is lifted by the small energy gap, $e^{-L^d/\xi}$, where L, d and ξ are a linear dimension of the finite system, dimensionality and a typical correlation length. For the topological ordered states with energy gaps, we may expect degeneracy of the ground states depending on the geometry of the system (topological degeneracy). When the system is finite, we expect edge states generically[13]. It implies the topological degeneracy is lifted by the energy gaps of the order $e^{-L/\xi}$.

2. Local Order Parameters of Quantum Liquids

After the first discovery of the fractional quantum Hall states, the quantum liquids have been recognized to exist quite universally in a quantum world where quantum effects can not be treated as a correction to the classical description and the quantum law itself takes the wheel to determine the ground state. The resonating valence bond (RVB) state which is proposed for a basic platform of the high-T_C superconductivity is a typical example[9]. The RVB state of the Anderson can be understood as a quantum mechanical collection of *local* spin singlets. When it becomes mobile under the doping, the state is expected to show superconductivity. Original ideas of this RVB go back to the Pauling's description of benzene compounds where the quantum mechanical ground state is composed of *local bonding states (covalent bonds)* where the basic variables to describe the state is not electrons localized at sites but the bonding states on links[10]. This is quite instructive. That is, in both of the Anderson's RVB and the Pauling's RVB, basic objects to describe the quantum liquids are quantum mechanical objects as a *singlet pair* and a *covalent bond*[1]. The "classical" objects as small magnets (localized spins) and electrons at site never play major roles. The constituents of the liquids themselves do not have a classical analogue and purely quantum mechanical objects. Based on this view point, it is natural to characterize these quantum objects, the singlet pairs and the covalent bonds, as working variables of the *local* quantum order parameters. It is to be compared with the conventional order parameter (a magnetic order parameter is defined by a local spin as a working variable). From these observations, we proposed to use quantized Berry phases to define local topological order parameters[1]. (We only treat here the singlet pairs as the topological order parameters. As for the local topological description by the covalent bonds, see ref.[1].) For example, there can be many kinds of quantum dimer states for frustrated Heisenberg models, such as column dimers, plaquette dimers, etc. As is clear, one can not find any classical local order parameters to characterize them. However, our topological order parameters can distinguish them as different phases not by just a crossover.

3. Quantized Berry Phases for the Topological Order Parameters of Frustrated Heisenberg Spins

Frustration among spins prevent from forming a magnetic order and their quantum ground states tend to belong to the quantum liquids without any symmetry breaking. Since they do not have any local order parameters, even if they have apparent different physical behaviors, it is difficult to make a clear distinction as a phase not just as a crossover. We apply the general scheme in the reference [1] to classify these frustrated spin systems. Defining quantized Berry phases as 0 or π, the spin liquids are characterized locally reflecting their topological order. We can distinguish many topological phases which are separated by local quantum phase transitions (local gap closings).

We consider following spin 1/2 Heisenberg models with general exchange couplings, $H = \sum_{ij} J_{ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j$. *We allow frustrations among spins.* We assume the ground state is *unique and gapped*. To define a local topological order parameter at a specific link $\langle ij \rangle$, we modify the exchange by making a local $SU(2)$ twist θ only at the link as

$$J_{ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j \to J_{ij}(\frac{1}{2}(e^{-i\theta} S_{i+} S_{j-} + e^{i\theta} S_{i-} S_{j+}) + S_{iz} S_{jz}).$$

Writing $x = e^{i\theta}$, we define a parameter dependent Hamiltonian $H(x)$ and its normalized ground state $|\psi(x)\rangle$ as $H(x)|\psi(x)\rangle = E(x)|\psi(x)\rangle$, $\langle\psi|\psi\rangle = 1$. Note that this Hamiltonian is invariant under the time-reversal (TR) Θ_T, $\Theta_T^{-1} H(x) \Theta_T = H(x)$[11]. Also note that by changing $\theta : 0 \to 2\pi$, we define a closed loop C in the parameter space of x.

Now we define the Berry connection as $A_\psi = \langle\psi|d\psi\rangle = \langle\psi|\frac{d}{dx}\psi\rangle dx$. Then the Berry phase along the loop C is defined as $i\gamma_C(A_\psi) = \int_C A_\psi$[12]. Besides that the system is gapped, we further assume *the excitation gap is always finite* (for $^\forall x$), to ensure the regularity of the ground state[3]. This may not be alway true, since the gap can collapse by the local perturbation as an appearance of localized states (edge states)[13]. Note that by changing a phase of the ground state as $|\psi(x)\rangle = |\psi'(x)\rangle e^{i\Omega(x)}$, the Berry connection gets modified as $A_\psi = A'_\psi + id\Omega$ [12, 3]. It is a gauge transformation. Then the Berry phase, $\boldsymbol{\gamma}_C$ also changes. It implies that the Berry phase is not well defined without specifying the phase of the ground state (the gauge fixing). It can be fixed by taking a single-valued reference state $|\phi\rangle$ and a gauge invariant projection into the ground state $P = |\psi\rangle\langle\psi| = |\psi'\rangle\langle\psi'|$ as $|\psi_\phi\rangle = P|\phi\rangle/\sqrt{N_\phi}$, $N_\phi = \|P|\phi\rangle\|^2 = |\eta_\phi|^2$, $\eta_\phi = \langle\psi|\phi\rangle$[3, 1]. We here require the normalization, N_ϕ, to be finite. When we use another reference state $|\phi'\rangle$ to fix the gauge, we have $|\psi_\phi\rangle = |\psi_{\phi'}\rangle e^{i\Omega}$, $\Omega = \arg(\eta_\phi - \eta_{\phi'})$. Due to this gauge transformation, the Berry phase gets modified as $\gamma_C(A_{\psi_\phi}) = \gamma_C(A_{\psi_{\phi'}}) + \Delta$, $\quad \Delta = \int_C d\Omega$. Since the reference states $|\phi\rangle$ and $|\phi'\rangle$ are single-valued on the C, the phase difference Ω is just different by $\Delta = 2\pi M_C$ with some integer M_C. Generically it implies that the Berry phase has a gauge invariant meaning just up to the integer as

$$\gamma_C \equiv -i \int_C A, \quad \mathrm{mod}\, 2\pi$$

By the TR invariance, the Berry phase get modified as $\gamma_C(A_\psi) = \sum_J C_J^* dC_j =$

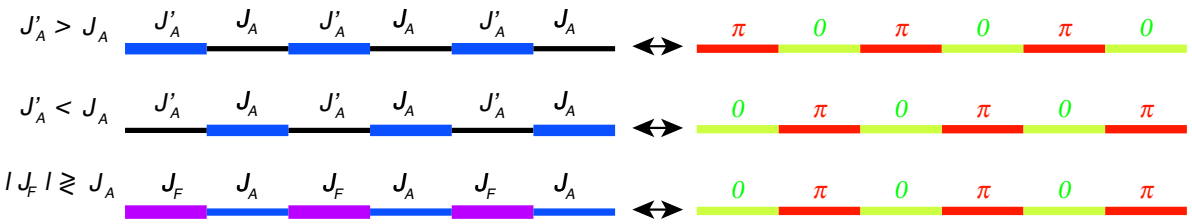

Figure 1. One dimensional Heisenberg models with alternating exchange interactions with periodic boundary condition (left). Numerically evaluated distribution of the quantized Berry phases (right). $J_A, J_{A'} > 0$ and $J_F < 0$. The results are independent of the system size. (We have checked a consistency of the results for various possible system sizes.)

$-\sum_J C_J dC_j^* = -\gamma_C(A_{\Theta\psi})$ since $\sum_J |C_J|^2 = 1$[1]. Therefore to be compatible with the gauge ambiguity, the Berry phase of the unique TR-invariant ground state, $|\psi\rangle \propto \Theta|\psi\rangle$, satisfies $\gamma_C(A_\psi) \equiv -\gamma_C(A_\psi) \pmod{2\pi}$. Then it is required to *be quantized* as

$$\gamma_C(A_\psi) = 0, \pi \pmod{2\pi}.$$

This quantized Berry phases have a topological stability since any small perturbations can not modify unless the gauge becomes singular. Here we note that the Berry phase of the singlet pair for the two site problem is π[1]. Now let us take any dimer covering of all sites $\mathcal{D} = \{\langle ij\rangle\}$ ($\#\mathcal{D} = N/2$, N is a total number od sites) and assume that the interaction is nonzero only on these dimer links, then the Berry phases, π, pickup the dimer pattern $\mathcal{D}$. Now imagine an adiabatic process to include interactions across the dimers. Due to the topological stability of the quantized Berry phase, they can not be modified unless the dimer gap collapses. This dimer limit presents a non-trivial pattern of a quantized Berry phase and shows the usefulness of the quantized Berry phases as *local order parameters of singlet pairs*. To show its real validity of the quantized Berry phases, we have diagonalized the Heisenberg Hamiltonians numerically by the Lanzcos algorithm and calculated the quantized Berry phases explicitly.

The first numerical examples are the Heisenberg chains with alternating exchanges. When the exchanges are both antiferromagnetic as $J_A > 0$ and $J_{A'} > 0$, it is a spin Pierls or dimerized chain. In this case, the Berry phases are π on the links with the strong exchange couplings and 0 on the one with the weak couplings (Fig.1). This is expected from the adiabatic principle and the quantization. When one of them is negative as $J_A > 0$ and $J_F < 0$, the calculated Berry phases are π for the antiferromagnetic links and 0 for the ferromagnetic ones. It is independent of the ratio J_A/J_F. Since the strong ferromagnetic limit is equivalent with the spin 1 chain, it is consistent with the topological nontrivial structure of the Haldane phases. Further analysis on the $S = 1$ systems will be published elsewhere. Next numerical examples are spin chains with nearest neighbor (NN) and next nearest neighbor (NNN) exchanges as ladder of triangles (Fig.2). These are typical systems with frustrations. (a) and (b) are two different but specific configurations where one may adiabatically connect the system with different

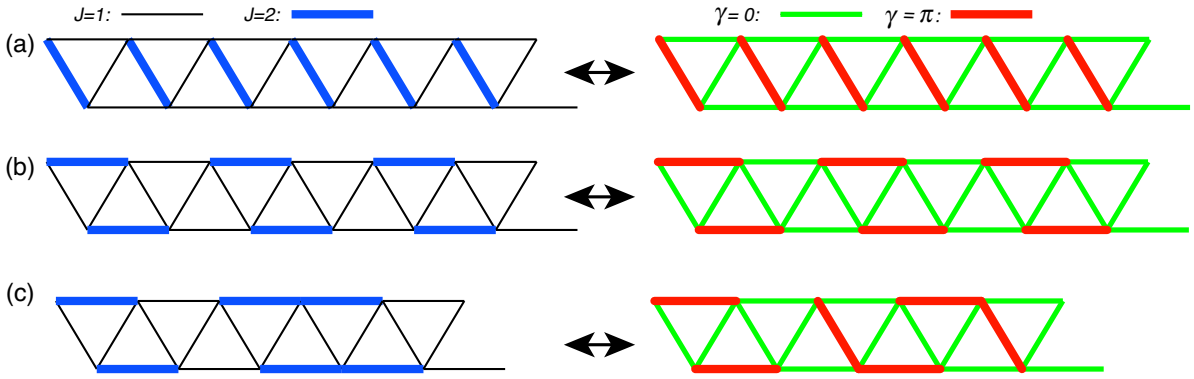

Figure 2. One dimensional Heisenberg models with NN and NNN exchanges (left) with periodic boundary condition. Numerically evaluated distribution of the quantized Berry phases (right). (a), (b) and (c): three different exchange configurations of $J = 1$ and $J' = 2$.

dimer coverings by the strong coupling bonds. In these cases, the quantized Berry phases are π for the strong coupling links and 0 for the rest links. This is consistent with the adiabatic principle. We note here that it is difficult to make a qualitative difference between the two quantum liquids by a conventional methods. However we have made a clear distinction between them as two different topological phases. The present scheme is not only valid for these simple situations but also useful for generic situation. For example, as for a system in the Fig.2 (c), we can not use the adiabatic principle simply. However the quantized Berry phases show non trivial behaviors and it make a clear distinction that the phase (c) is topologically different from the ones in the (a) and (b) as an independent phase not just as a crossover. A local quantum phase transition separates them by the gap closing. As is now clear, the present scheme is quite powerful to make a local characterization of the topological quantum insulators.

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